

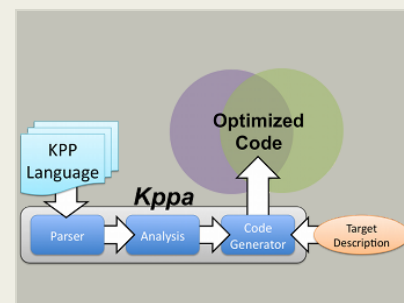
A High Performance Chemical Simulation Preprocessor and Source Code Generator, Phase I

Completed Technology Project (2014 - 2014)



Project Introduction

Numerical simulations of chemical kinetics are a critical component of aerospace research, Earth systems research, and energy research. These simulations enable a better understanding of the evolution of chemical species over time in domains as diverse as climate and weather prediction, combustion simulation, and air quality prediction. The time-to-solution in these simulations can be improved by over 30X via computational accelerators like Graphical Processing Units (GPUs) or the Intel Xeon Phi coprocessor, but the state-of-the-art tools for chemical kinetics do not support accelerators. ParaTools will develop a code generation tool called "Kppa" into a production-grade product that translates a high-level description of a chemical reaction network into simulation code that supports computational accelerators to significantly reduce time-to-solution. The generated code will provide the same software interface as existing tools to ensure immediate compatibility with popular codes like GEOS-Chem, WRF-Chem, MCM, etc. Kppa will include an online user productivity environment called "Kppa Cloud" for the development, testing, and benchmarking of chemical simulation codes. Kppa Cloud will enable users to graphically formulate new chemical reaction networks, maintain a library of chemical mechanisms, develop new mechanisms collaboratively, generate simulation code, explore the computational and numerical characteristics of the generated code, and test the generated code for stability and correctness. Kppa will enable supercomputer-level performance on smaller computers with lower costs, lower barriers to entry, and enable the rapid creation of high-performance kinetics simulations. Kppa will build on open source technologies to be backward compatible with the state-of-the-art in modeling and simulation and employ a modular design enabling extensibility to the computer architectures of the future.



A High Performance Chemical Simulation Preprocessor and Source Code Generator Project Image

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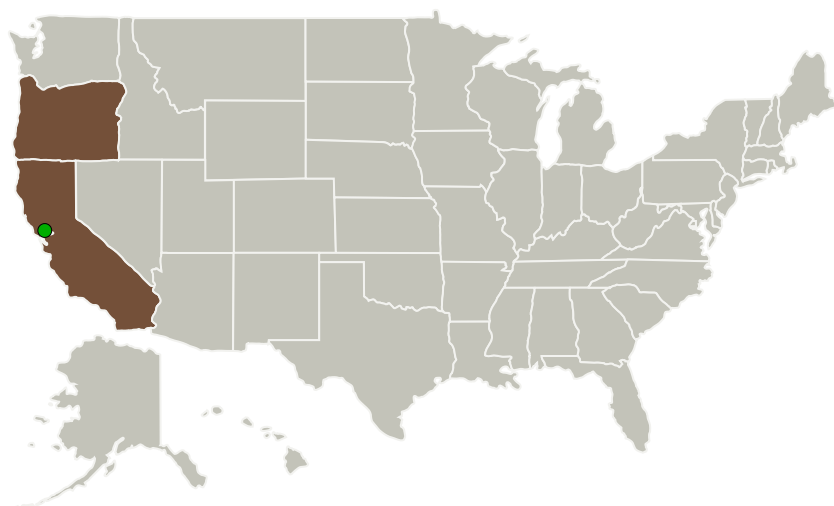
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Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
ParaTools, Inc.	Lead Organization	Industry	Eugene, Oregon
● Ames Research Center(ARC)	Supporting Organization	NASA Center	Moffett Field, California

Primary U.S. Work Locations

California	Oregon
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Project Transitions



June 2014: Project Start



December 2014: Closed out

Closeout Documentation:

- Final Summary Chart(<https://techport.nasa.gov/file/137505>)

Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

Lead Organization:

ParaTools, Inc.

Responsible Program:

Small Business Innovation Research/Small Business Tech Transfer

Project Management

Program Director:

Jason L Kessler

Program Manager:

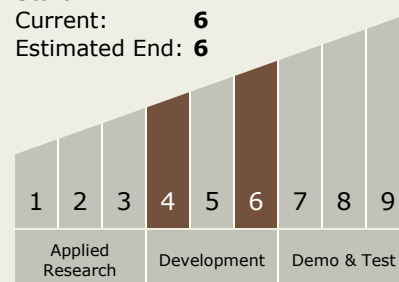
Carlos Torrez

Principal Investigator:

John C Linford

Technology Maturity (TRL)

Start: **4**
Current: **6**
Estimated End: **6**

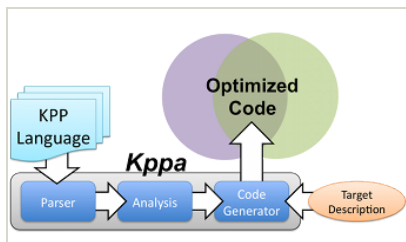


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Images



Project Image

A High Performance Chemical Simulation Preprocessor and Source Code Generator Project Image

(<https://techport.nasa.gov/image/135753>)

Technology Areas

Primary:

- TX11 Software, Modeling, Simulation, and Information Processing
 - └ TX11.1 Software Development, Engineering, and Integrity
 - └ TX11.1.1 Tools and Methodologies for Software Design and Development

Target Destinations

The Moon, Mars, Outside the Solar System, The Sun, Earth, Others Inside the Solar System